10-664-165

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      6 DEC 01
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        DEC 09
                 12 databases to be removed from STN on December 31, 2004
NEWS
     7
        DEC 15
NEWS
                 MEDLINE update schedule for December 2004
NEWS
        DEC 17
                 ELCOM reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
     10 DEC 17
                 COMPUAB reloaded; updating to resume; current-awareness
NEWS
                 alerts (SDIs) affected
NEWS
     11 DEC 17
                 SOLIDSTATE reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
NEWS
     12 DEC 17
                 CERAB reloaded; updating to resume; current-awareness
                 alerts (SDIs) affected
                 THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS
     13 DEC 17
NEWS
     14 DEC 30
                 EPFULL: New patent full text database to be available on STN
                 CAPLUS - PATENT COVERAGE EXPANDED
NEWS
     15 DEC 30
NEWS
     16 JAN 03
                 No connect-hour charges in EPFULL during January and
                 February 2005
NEWS
     17 JAN 11
                 CA/CAPLUS - Expanded patent coverage to include Russia
                 (Federal Institute of Industrial Property)
NEWS EXPRESS
              JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT
              MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
              AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
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              CAS World Wide Web Site (general information)
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=> file registry
COST IN U.S. DOLLARS

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FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 11 JAN 2005 HIGHEST RN 811782-89-5 DICTIONARY FILE UPDATES: 11 JAN 2005 HIGHEST RN 811782-89-5

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\STNEXP4\QUERIES\10664165.str

L1 STRUCTURE UPLOADED

=> d l1

G1 C, H, O, S, N

L1 HAS NO ANSWERS

10458286

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full FULL SEARCH INITIATED 15:14:56 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 14.5% PROCESSED 252338 ITERATIONS (1 INCOMPLETE) 3115 ANSWERS

< 20.4% PROCESSED 354173 ITERATIONS (1 INCOMPLETE) 4837 ANSWERS

< 23.1% PROCESSED 400000 ITERATIONS (1 INCOMPLETE) 5511 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.41

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**

PROJECTED ITERATIONS: EXCEEDS 1000000 PROJECTED ANSWERS: EXCEEDS 23432

L2 5511 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
162.40

FILE 'CAPLUS' ENTERED AT 15:16:00 ON 13 JAN 2005 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

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FILE COVERS 1907 - 13 Jan 2005 VOL 142 ISS 3 FILE LAST UPDATED: 12 Jan 2005 (20050112/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 12

L3 615 L2

=> s l3 and sodium 961054 SODIUM

L4 35 L3 AND SODIUM

=> s l3 and channels 138103 CHANNELS

L5 1 L3 AND CHANNELS

=> s 13 and "cell membrane"

CODEN: PIXXD2

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1863637 "CELL"
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                  (BLOOD (W) VESSEL)
L7
            11 L3 AND BLOOD VESSEL
=> s 12 full
           615 L2
L8
=> s 18 and bladder
         29744 BLADDER
L9
             8 L8 AND BLADDER
=> s 18 and bronchial tube
         14877 BRONCHIAL
        292134 TUBE
            36 BRONCHIAL TUBE
                  (BRONCHIAL (W) TUBE)
L10
             0 L8 AND BRONCHIAL TUBE
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        292134 TUBE
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L11
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       1863637 CELL
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                  (NEURONAL (W) CELL)
L12
             0 L8 AND NEURONAL CELL
=> s 18 and gastroinstestinal tract
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             1 GASTROINSTESTINAL TRACT
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             0 L8 AND GASTROINSTESTINAL TRACT
L13
=> s 15 or 16 or 17 or 19
            19 L5 OR L6 OR L7 OR L9
=> d bib abs 114
L14 ANSWER 1 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
     2004:927010 CAPLUS
AN
DN
     141:376382
TI
     Pin1-modulating compounds and methods of use for the treatment of
     Pin1-associated diseases, including cancer
     Bao, Lere; Kimzey, Amy
IN
PA
     Pintex Pharmaceuticals, Inc., USA
     PCT Int. Appl., 189 pp.
so
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DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                        KIND
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                                          APPLICATION NO.
                                                                  DATE
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     WO 2004093803
                         A2
                                20041104 WO 2004-US11957
рT
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             TD, TG
PRAI US 2003-463271P
                          Ρ
                                20030416
     The invention is directed to modulators, e.g., inhibitors, of Pin1 and
     Pin1-related proteins and the use of such modulators for treatment of Pin1
     associated states, e.g., for the treatment of cancer. The present invention
     aims to provide photochemotherapeutic compds. with increased specificity
     as compared with known agents.
=> s bib abs 1-19 hitstr 114
MISSING OPERATOR HITSTR L14
The search profile that was entered contains terms or
nested terms that are not separated by a logical operator.
=> d bib abs 1-19 hitstr 114
L14
     ANSWER 1 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
AN
     2004:927010 CAPLUS
DN
     141:376382
TΙ
     Pin1-modulating compounds and methods of use for the treatment of
     Pin1-associated diseases, including cancer
     Bao, Lere; Kimzey, Amy
IN
PA
     Pintex Pharmaceuticals, Inc., USA
     PCT Int. Appl., 189 pp.
so
                                                                              NPA
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                                           APPLICATION NO.
     PATENT NO.
                         KIND
                                DATE
                                                                  DATE
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PΙ
    WO 2004093803
                         A2
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             TD, TG
PRAI US 2003-463271P
                          Ρ
                                20030416
     The invention is directed to modulators, e.g., inhibitors, of Pin1 and
```

Pinl-related proteins and the use of such modulators for treatment of Pinl associated states, e.g., for the treatment of cancer. The present invention

aims to provide photochemotherapeutic compds. with increased specificity as compared with known agents.

IT 676649-27-7

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

RN 676649-27-7 CAPLUS

CN 3-Thiazolidinebutanoic acid, 5-[(1,2,3,4,4a,9,10,10a-octahydro-6,7-dimethoxy-3-methyl-2-phenanthrenyl)methylene]-4-oxo-2-thioxo-(9CI) (CA INDEX NAME)

MeO
$$\sim$$
 CH \sim S \sim S \sim MeO \sim (CH₂)₃-CO₂H

L14 ANSWER 2 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:792843 CAPLUS

DN 141:421217

TI Effects of modification at the fifth residue of μ -conotoxin GIIIA with bulky tags on the electrically stimulated contraction of the rat diaphragm

AU Nakamura, M.; Ishida, Y.; Kohno, T.; Sato, K.; Oba, Y.; Nakamura, H.

CS Graduate School of Bioagricultural Sciences, Nagoya University, Nagoya, 464-8601, Japan

SO Journal of Peptide Research (2004), 64(3), 110-117 CODEN: JPERFA; ISSN: 1397-002X

PB Blackwell Publishing Ltd.

DT Journal

LA English

AB μ -Conotoxin GIIIA, a peptide toxin from the cone snail, blocks muscle-type sodium **channels**. Thr 5 of μ -conotoxin GIIIA, located on the opposite side of the active site in the globular mol., was replaced by Cys to which the bulky tags were attached. The tagged μ -conotoxin GIIIA derivs., except for the phospholipid-tagged one, exerted the biol. activity with a potency slightly weaker than natural μ -conotoxin GIIIA. When the biotinylated tags of various lengths were added, the presence of avidin suppressed the action of the biotinylated toxins of <4 nm, but not with 5 nm. The bulky biotinylated tags are useful as a caliper to measure the depth of receptor sites in the **channels**.

IT 795300-38-8P

RL: ADV (Adverse effect, including toxicity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (effects of modification at the fifth residue of μ -conotoxin GIIIA with bulky tags on the elec. stimulated contraction of the rat diaphragm)

RN 795300-38-8 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RE.CNT 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

NPA

```
AN
     2004:566563 CAPLUS
DN
     141:123479
TI
     Preparation of N-aryl benzamides as histone deacetylase inhibitors
IN
     Schuppan, Detlef; Herold, Christoph; Gansmayer, Marion; Ocker, Matthias;
     Thierauch, Karl-Heinz
PA
     Schering Aktiengesellschaft, Germany
     PCT Int. Appl., 249 pp.
SO
     CODEN: PIXXD2
DT
     Patent
     English
LA
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                            APPLICATION NO.
                                                                    DATE
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     WO 2004058234
                          A2
                                20040715
                                            WO 2003-EP14071
                                                                    20031211
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             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,
             NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,
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PRAI EP 2002-90431
                                20021227
                          Α
     EP 2003-90061
                          Α
                                20030312
os
    MARPAT 141:123479
GI
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$$\begin{array}{c|c} \text{A-X-Q-(CH_2)} & & & \\ \text{R}^1 & & & \\ & & \text{H} & & \\ & & & \\$$

NPA

AB Histone deacetylase inhibitors I [A = (un)substituted Ph or heterocycle; X = bond, alkyl, alkyloxyalkyl, alkylthioalkyl, etc.; Q = amide, urea, amidoester, etc.; n = 0-4 provided that when X = bond, n is not 0; R1 and R2 independently = H, halo, OH, amino, alkyl, etc.; R3 = OH or amino] and their pharmaceutically acceptable salts are prepared and disclosed as agents to be used in pharmaceutical combinations with phthalazine or pyridazine derivs. (disclosed in prior patent WO 98/35958) which are known angiogenesis inhibitors. Thus, e.g., II was prepared via coupling reaction of 3-pyridinemethanol, N,N'-carbonyldiimidazole and 4-aminomethyl-N-[2-(N-tertbutoxycarbonyl)aminophenyl]benzamide with subsequent removal of N-BOC

IT

group. II was combined with tamoxifen and the VEGF receptor antagonist 1-(4-chloroanilino)-4-(pyridylmethyl)phthalazine hydrochloride and this pharmaceutical composition was evaluated in a colorectal carcinoma model in Waq rats. The results of the model study indicated the combination therapy significantly restricted tumor growth relative to the reference (2 ± 0.5% tumor volume) and the individual application of each compound 722547-82-2

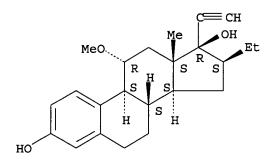
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of N-arylbenzamides as histone deacetylase inhibitors)

722547-82-2 CAPLUS RN

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,17-diol, 16-ethyl-11-methoxy-, $(11\alpha, 16\beta, 17\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ANSWER 4 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN L14

AN2004:513479 CAPLUS

DN 141:71736

ΤI Isolation and preparation of diterpenoids, compositions thereof, and their use as anticancer or antifungal agents

IN Beauparlant, Pierre; Attardo, Giorgio; Zhang, Zhiying; Stafford, Angela M.; Ubillas, Rosa; Mcalpine, James B.

PA Gemin X Biotechnologies Inc., Can.; Galileo Pharmaceuticals, Inc.; Fortin, Samuel; Tripathy, Sasmita

NPA

PCT Int. Appl., 185 pp. SO

CODEN: PIXXD2

DTPatent

LA English

FAN.	CNT	1																	
	PATENT NO.						D :	DATE		APPLICATION NO.						DATE			
ΡI	WO 2004052282				A2 20040624				1	WO 2	003-1	US38	20031204						
	WO	2004	0522	82		A3 20041007													
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			TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
PRAI	US	2002	-431	096P		₽		2002	1205										
os	MAI	RPAT	141:	7173	6														

MARPAT 141:71736

GI

$$R^9$$
 R^7
 R^7

AB The present invention relates to diterpenoids I [Q1, Q2 = O, S, NH, NNHR; R = H, C1-10-alkyl, aryl; Q3 = O, S, N(H); R1, R2 = H, halogen, NH2, C1-10-alkyl, C1-10-alkoxy, C1-10-hydroxyalkyl, C1-10-aminoalkyl, C1-10-haloalkyl, , C2-10-alkenyl, C2-10-alkynyl, , C1-10-alkyl, C3-7-cycloalkyl, aryl , C1-10-arylalkyl, 3- to 7-membered heterocycle; CR1R2 = C3-7-cycloalkyl; A = N, CR3; B = N, CR4; D = N, CR5; E = N, CR6 (with the proviso that one of A, B, D, E = CR3, CR4, CR5, CR6); R3, R4, R5, R6 = H, halo, CN, NH2, NO2, CO2H, CONH2, SH, SONH2, SO2NH2, C1-10-oxyalkyl, C1-10-alkyl, C1-10-alkoxy, C1-10-hydroxyalkyl, C1-10-aminoalkyl, C1-10-haloalkyl, C2-10-alkenyl, C2-10-alkynyl, C3-7-cycloalkyl, aryl, C1-10-arylalkyl, 3- to 7-membered non-aromatic heterocycle, 5- to 7-membered aromatic heterocycle, etc.; R3C:CR4, R5C:CR6, R4C:CR5 = C3-7-cycloalkenyl, 5- to 7-membered (non)aromatic heterocycle; R7 = H, C1-10-alkyl, C1-10-alkoxy; R8, R9 = H, halo, CN, NH2, NO2, CO2H, CONH2, SH, SONH2, SO2NH2, C1-10-oxyalkyl, C1-10-alkyl, C1-10-alkoxy, etc.; R10 = H, C1-10-alkyl, C3-7-cycloalkyl, C0-(C1-10-alkyl), C1-10-oxyalkyl, CONH2, CONHR12, aryl; R12 = C1-10-alkyl; halo = F, Cl, Br, I], compns. comprising an effective amount of I, and methods useful for treating or preventing cancer or a neoplastic disorder comprising administering an effective amount The compds., compns., and methods of the invention are also useful for inhibiting the growth of a cancer cell or neoplastic cell, or for inducing apoptosis in a cancer or neoplastic cell. The compds., compns., and methods of the invention are further useful for treating or preventing a fungal infection. The compds., compns., and methods of the invention are also useful for inhibiting the growth of a fungus. Podocarpane diterpene II was isolated from Linum arboretum. The effect of II on cancer-cell viability was studied; capases were activated in cancer cell lines H1299 and C33A following 16 h incubation with 1.6 \(\mu \) of I showing selective apoptosis in cancer cells.

OMe

Me

II

IT 709667-53-8P

RN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and enol silylation of; isolation and preparation of diterpenoids,

compns. thereof, and their use as anticancer or antifungal agents) 709667-53-8 CAPLUS

CN 2(1H)-Phenanthrenone, 3,4,4a,9,10,10a-hexahydro-6-methoxy-1,1,4a-trimethyl-, (4aR,10aR)- (9CI) (CA INDEX NAME)

IT 709667-52-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

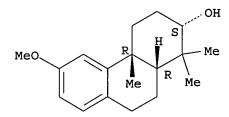
(preparation and oxidation of; isolation and preparation of diterpenoids, compns.

thereof, and their use as anticancer or antifungal agents)

RN 709667-52-7 CAPLUS

CN 2-Phenanthrenol, 1,2,3,4,4a,9,10,10a-octahydro-6-methoxy-1,1,4a-trimethyl-, (2S,4aR,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 709667-21-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, selenenylation and oxidative deselenation of; isolation and preparation of diterpenoids, compns. thereof, and their use as anticancer or antifungal agents)

RN 709667-21-0 CAPLUS

CN 2(1H)-Phenanthrenone, 3,4,4a,9,10,10a-hexahydro-6-methoxy-1,4a-dimethyl-, (1R,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L14 ANSWER 5 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:291950 CAPLUS

DN 140:315042

NATA

- Pin1-modulating compounds and methods of use for the treatment of ТT Pin1-associated diseases, including cancer
- IN Mckee, Timothy D.; Suto, Robert K.; Tibbitts, Thomas; Sowadski, Janusz
- PA Pintex Pharmaceuticals, Inc., USA
- SO PCT Int. Appl., 166 pp.

CODEN: PIXXD2

DTPatent

LA English

FAN.CNT 1

L MIN .	CMT	Τ.																	
	PATENT NO.						IND DATE				APPL		DATE						
																			
ΡI	WO	2004	0285	35		A1		20040408		1	WO 2	003-1	20030303						
		W:	ΑE,	AG,	AL,	AM,	AT,	ΑU,	ΑZ,	BA,	BB,	ВG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
			CO,	CR,	CU,	CZ,	DΕ,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,	
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,	
			PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,	
			UA,	UG,	UΖ,	VC,	VN,	ΥU,	ZA,	ZM,	zw								
		RW:	GH,	GM,	KΕ,	LS,	MW,	MZ,	SD,	SL,	SZ,	ΤZ,	ŪĠ,	ZM,	ZW,	AM,	ΑZ,	BY,	
			KG,	ΚZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,	
			FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	RO,	SE,	SI,	SK,	TR,	
			BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG	
	US 2004214872									1	US 2	003-							
PRAI	US	S 2002-414077P						2002	0926										

os MARPAT 140:315042

AΒ The invention is directed to modulators, e.g., inhibitors, of Pin1 and Pin1-related proteins and the use of such modulators for treatment of Pin1 associated states, e.g., for the treatment of cancer. Synthetic methods are included.

IT 676649-27-7

> RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(Pin1-modulating compds. for treatment of Pin1-associated diseases, including cancer)

RN676649-27-7 CAPLUS

3-Thiazolidinebutanoic acid, 5-[(1,2,3,4,4a,9,10,10a-octahydro-6,7-CN dimethoxy-3-methyl-2-phenanthrenyl)methylene]-4-oxo-2-thioxo- (9CI) (CA INDEX NAME)

MeO
$$\sim$$
 CH \sim S \sim S \sim MeO \sim (CH₂)₃-CO₂H

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L14 ANSWER 6 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
- 2004:220882 CAPLUS AN
- DN 141:289239
- ΤI Influence of Estrogen Cytostatics on Activity of Plasma Membrane Enzymes 5'-Nucleotidase and N+-K+-ATPase
- ΑU Mayatskaya, E. E.; Semeikin, A. V.; Rzheznikov, V. M.; Shimanovskii, N. L.
- CS Research Center for Endocrinology, Department of Molecular Pharmacology and Radiobiology, Russian State Medical University, USA
- Bulletin of Experimental Biology and Medicine (Translation of Byulleten SO

TΥ

Eksperimental'noi Biologii i Meditsiny) (2003), 136(6), 557-559 CODEN: BEXBAN; ISSN: 0007-4888

PB Kluwer Academic/Consultants Bureau

DT Journal

LA English

AB The authors studied the effect of four conjugated synthetic derivs. of estrone and ethynylestradiol and bis-β-chloroethylamine-containing substance on activity of plasma membrane enzymes 5'-nucleotidase and N+-K+-ATPase. As differentiated from precursors, estrogen cytostatics decreased activity of plasma membrane enzymes. Reference prepns. chlorophenacyl and estradiol had little effect on activity of 5'-nucleotidase and N+-K+-ATPase. These data suggest that damage to plasma membrane enzymes is related to the effect of estrogen cytostatic mols. Test compds. produced an antiproliferative effect on estrogen-independent tumor cells, which strongly correlated with a decrease in activity of plasma membrane enzymes 5'-nucleotidase and N+-K+-ATPase. The derivative of ethynylestradiol with the cytostatic residue in the 3-position of the steroid nucleus (Po-714-11a) most significantly modulated enzyme activity.

458569-13-6 458569-15-8 762303-31-1 762303-32-2

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(influence of estrogen cytostatics on activity of plasma membrane enzymes 5'-nucleotidase and N+-K+-ATPase)

RN 458569-13-6 CAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,11,17-triol, 17-acetate 3-[[4-[bis(2-chloroethyl)amino]phenyl]acetate] 11-formate, $(11\alpha,17\alpha)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 458569-15-8 CAPLUS

CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,11,17-triol, 11,17-diacetate 3-[[4-[bis(2-chloroethyl)amino]phenyl]acetate], $(11\alpha,17\alpha)$ - (9CI) (CA INDEX NAME)

10458286

RN 762303-31-1 CAPLUS

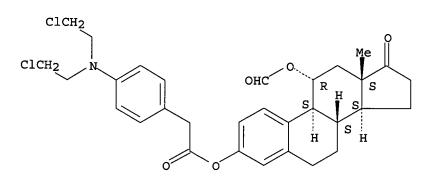
CN 19-Norpregna-1,3,5(10)-trien-20-yne-3,11,17-triol, 17-acetate 3-[4-[bis(2-chloroethyl)amino]benzeneacetate], $(11\alpha,17\alpha)$ -(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 762303-32-2 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 3-[[[4-[bis(2-chloroethyl)amino]phenyl]acety 1]oxy]-11-(formyloxy)-, (11 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 7 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:220333 CAPLUS

DN 140:270854

TI Preparation of 1,3,8-triazaspiro[4.5]decan-4-ones for the treatment of ORL-1 receptor mediated disorders

IN Battista, Kathleen; Bignan, Gilles; Connolly, Peter J.; Reitz, Allen B.;
Morgan Ross, Tina; Scott, Malcolm; Middleton, Steve A.; Orsini, Michael

NPA

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PA
    Janssen Pharmaceutica, N.V., Belg.
    PCT Int. Appl., 249 pp.
    CODEN: PIXXD2
DT
    Patent
LA
    English
FAN.CNT 1
    PATENT NO.
                       KIND DATE
                                         APPLICATION NO.
                                                                 DATE
                                                                 _____
    WO 2004022558
                        A2
                               20040318 WO 2003-US27956
                                                                 20030905
PΤ
                               20040521
    WO 2004022558
                        A3
        W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
            CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
            GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
            LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
            PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
            TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
        RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
            KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
            FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
            BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
                               20040722 US 2003-656934
    US 2004142955
                         A1
                                                                 20030905
                                           BR 2003-6309
    BR 2003006309
                         Α
                               20041019
                                                                  20030905
PRAI US 2002-409134P
                         Ρ
                               20020909
                         W
    WO 2003-US27956
                               20030905
    MARPAT 140:270854
OS
GΙ
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
AB
    Title compds. I [R0 = CRaRbCOHRa-(CRcRd)1-3X, (CRcRd)1-3COHRaCRaRbX; Ra,
    Rb = H, alkyl; Rc, Rd = H, OH, carboxy, etc.; X = NR1R2, CONR1R2, NR1,
    etc.; R1, R2 = H, alkyl, alkoxy, etc.; R3 = aryl, arylalkyl, heteroaryl,
    etc.; A = (R4)n; R4 = OH, alkyl, alkyl-OH; n = 0-2; B = (L1)m; L1 = alkyl,
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alkenyl with provisos; m = 0-1; C = (R5)p and (R6)q substituted cycloalkyl, partially unsatd. carbocyclyl (sic), aryl, etc.; R5 = OH, carboxy, halo, etc.; p = 0-5; R6 = (L2)0-1R7; q = 0-1; L2 = alkyl, alkenyl, alkynyl, etc.; R7 = aryl, partially unsatd. carbocyclyl, cycloalkyl, etc.] and their pharmaceutically acceptable salts were prepared For example, amination of epoxide II, e.g., prepared from cyclooctanecarboxaldehyde in 2-steps, with 4-aminopyridine afforded amino alc. III. In human ORL-1 receptor binding affinity assays, approx. 470-examples of compds. I exhibited IC50 values ranging from 0.10 ->10,000 nM, e.g., the IC50 value of triazaspiro[4.5]decan-4-one III was 8.73 nM. Compds. I are claimed useful for the treatment of anxiety, depression, migraine, etc..

IT 674789-13-0P

CN

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(drug target; preparation of triazaspiro[4.5]decan-4-ones for the treatment of ORL-1 receptor mediated disorders)

RN674789-13-0 CAPLUS

> 1,3,8-Triazaspiro[4.5]decan-4-one, 3-[(2S)-2-hydroxy-3-[[[(1R,4aS,10aR)-1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-1phenanthrenyl]methyl]amino]propyl]-1-phenyl-8-[2-[2-(2thienyl)phenyl]ethyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

IT 674478-64-9P 674789-14-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of triazaspiro[4.5]decan-4-ones for the treatment of ORL-1 receptor mediated disorders)

RN 674478-64-9 CAPLUS

CN 1,3,8-Triazaspiro[4.5]decan-4-one, 8-cyclooctyl-1-(4-fluorophenyl)-3-[(2R)-2-hydroxy-3-[[(1S,4aR,10aS)-1,2,3,4,4a,9,10,10a-octahydro-1,4a-dimethyl-7-(1-methylethyl)-1-phenanthrenyl]methyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 674789-14-1 CAPLUS

CN 1,3,8-Triazaspiro[4.5]decan-4-one, 8-(1,2-dihydro-1-acenaphthylenyl)-1-(4-fluorophenyl)-3-[(2S)-2-hydroxy-3-[[[(1R,4aS,10aR)-1,2,3,4,4a,9,10,10a-

octahydro-1,4a-dimethyl-7-(1-methylethyl)-1-phenanthrenyl]methyl]amino]propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 8 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:182541 CAPLUS

DN 140:229476

TI Treatment of dyspareunia with topically administered nitroglycerin formulations

IN Place, Virgil A.; Wilson, Leland F.; Doherty, Paul C.; Hanamoto, Mark S.; Spivack, Alfred P.; Gesundheit, Neil; Bennett, Sean R.; Doherty, Jane K.

PA USA

SO U.S. Pat. Appl. Publ., 18 pp., Cont.-in-part of U.S. Ser. No. 905,458. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 6

L'ETTA .	CNIO				/
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
ΡI	US 2004044080	A1	20040304	US 2003-407858	20030404
	US 5877216	A	19990302	US 1997-959064	19971028
	US 6306841	B1	20011023	US 2000-539484	20000330
	US 2001051656	A1	20011213	US 2001-905458	20010713
	US 6593313	B2	20030715		
PRAI	US 1997-959057	B2	19971028		
	US 1997-959064	A2	19971028		
	US 1998-181316	B1	19981027		
	US 2000-539484	A1	20000330		
	US 2001-905458	A2	20010713		
				_	

AB Methods and formulations for treating dyspareunia are provided. A pharmaceutical composition formulated so as to contain a therapeutically effective amount of nitroglycerin is administered to the vagina or vulvar area of the individual undergoing treatment. Preferred formulations are immediate release formulations in which at least 80% of the nitroglycerin in the formulation is released therefrom within 4 h following administration. The formulations may contain one or more addnl. active agents, e.g., agents that are also useful to treat dyspareunia and/or potentiate the action of nitroglycerin. Such addnl. agents include vasoactive agents such as prostaglandins, phosphodiesterase inhibitors, androgens such as testosterone, estrogens such as estradiol, and selective modulators of estrogen and androgen receptors. A kit for a patient to use in the self-administration of the formulation is also provided.

IT 666702-84-7

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (selective estrogen receptor modulator, as addnl. active agent; dyspareunia treatment with topically administered nitroglycerin formulations)

RN 666702-84-7 CAPLUS

CN Estra-1,3,5(10)-triene-7-undecanamide, N-butyl-3,17-dihydroxy-N-methyl-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 9 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:828852 CAPLUS

DN 140:139694

TI The effects of 2-methoxy oestrogens and their sulphamoylated derivatives in conjunction with TNF- α on endothelial and fibroblast cell growth, morphology and apoptosis

AU Ho, Y. T.; Newman, S. P.; Purohit, A.; Leese, M. P.; Potter, B. V. L.; Reed, M. J.

CS Faculty of Medicine, Endocrinology and Metabolic Medicine and Sterix Ltd., Imperial College, St. Mary's Hospital, London, W2 1NY, UK

SO Journal of Steroid Biochemistry and Molecular Biology (2003), 86(2), 189-196

CODEN: JSBBEZ; ISSN: 0960-0760

PB : Elsevier Science Ltd.

DT Journal

LA English

AB

2-Methoxyoestradiol (2-MeOE2) is a potent anti-angiogenic agent. Its 3and 17-sulfamoylated derivs. have been demonstrated to induce G2-M cell cycle arrest and apoptosis in breast cancer cells in vitro as well as tumor regression in rats in vivo with greater potency than the parent estrogen. To determine whether the anti-cancer properties of these derivs. can be synergistically enhanced with low-dose TNF- α co-treatment, the authors investigated the effects of these treatments in adult human fibroblasts and human umbilical vein endothelial cells (HUVECs). Treatment of fibroblasts with 0.1 µM 2-methoxyoestradiol-3,17-bis sulfamate (2-MeOE2bisMATE) but not 2-MeOE2 caused a reversible morphol. change and induced G2-M arrest (from 12 to 33%) but not subsequent apoptosis. In contrast, treatment of HUVECs did not induce morphol. change or G2-M arrest. Using a nucleosomal ELISA assay, the authors showed that TNF- α (20 ng/mL) combination treatment synergistically increases 0.1 μM 2-MeOE2bisMATE-induced but not 0.1 μM 2-MeOE2-induced apoptosis in HUVECs. These results suggest that $TNF-\alpha$ co-treatment may be a beneficial method of increasing the potency of 2-substituted estrogens as anti-angiogenic agents through synergistic induction of apoptosis in endothelial cells while maintaining

low cytotoxicity to fibroblasts.

IT 401600-86-0

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (effects of 2-methoxy estrogens and their sulfamoylated derivs. in conjunction with TNF- α on human vascular endothelial and dermal fibroblast cell growth, morphol. and apoptosis)

RN 401600-86-0 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, disulfamate, (17 β)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 10 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN (2003:7)19252 CAPLUS

DN \ 139:22/4972

TI Synthesis of 2-methoxyestradiol derivatives and uses as antiangiogenic agents

IN Lavallee, Theresa M.; Pribluda, Victor S.; Simons, Jonathan; Mabjeesh, Nicola; Giannakakou, Paraskevi

NPA

PA Entremed, Inc., USA

SO PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN CNT 1

FAN.	CNT	T																		
	PATENT NO.)	DATE		2	APPL	ICAT		DATE						
							-										. <u></u>			
ΡI	WO 2003073985				A2		2003	0912	1	WO 2	003-1		20030227							
	WO	2003	0739	85		A3		20031231												
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,		
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,		
			LS,	LT,	LU,	LV,	ΜA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,		
			PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,		
			ΤZ,	UA,	ŪĠ,	US,	UZ,	VC,	VN,	ΥU,	ZA,	ZM,	ZW							
		RW:	GH,	GM,	KE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,		
			KG,	ΚZ,	MD,	RU,	ТJ,	TM,	ΑT,	BE,	ВG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,		
			FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	SK,	TR,	BF,	ВJ,	CF,		
			CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NΕ,	SN,	TD,	TG					
PRAI	US	2002	-3612	267P		P		2002	0301											

AB Compns. and methods for treating mammalian disease characterized by undesirable angiogenesis and for controlling a number of angiogenesis-related events, conditions, or substances, by administering derivs. of

 $2\mbox{-methoxyestradiol}$ of general formula (I) wherein the variables are defined in the specification.

IT 431901-79-0 431901-81-4 431901-84-7

431901-85-8 431901-89-2

RL: RCT (Reactant); RACT (Reactant or reagent)
 (synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic
 agents)

RN 431901-79-0 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 16-(2-butenyl)-2-methoxy-3-(phenylmethoxy)-, (16α) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 431901-81-4 CAPLUS

CN Estra-1,3,5(10)-triene-16-carboxylic acid, 2-methoxy-17-oxo-3-(phenylmethoxy)-16-(2-propenyl)-, methyl ester, (16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431901-84-7 CAPLUS

CN Estra-1,3,5(10)-triene-16-carboxylic acid, 2-methoxy-17-oxo-3-(phenylmethoxy)-, methyl ester, (16β)- (9CI) (CA INDEX NAME)

RN 431901-85-8 CAPLUS CN Estra-1,3,5(10)-trien-17-ol, 16-(2-butenyl)-2-methoxy-3-(phenylmethoxy)-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 431901-89-2 CAPLUS CN Estra-1,3,5(10)-trien-3-ol, 2-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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IT
     431901-68-7P 431901-69-8P 431901-70-1P
     431901-71-2P 431901-72-3P 431901-77-8P
     431901-78-9P 431901-80-3DP, alkyl derivs.
     431901-89-2DP, alkyl analogs 431901-90-5P
     431901-91-6P 431901-92-7P 431901-93-8P
     431901-98-3P 431901-99-4P 431902-01-1P
     431902-02-2P 431902-03-3P 431902-04-4P
     431902-05-5P 431902-06-6P 438044-30-5P
     464924-32-1P 594873-85-5P 594873-86-6P
     594873-87-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (synthesis of 2-methoxyestradiol derivs. and uses as antiangiogenic
        agents)
RN
     431901-68-7 CAPLUS
     Estra-1,3,5(10)-trien-3-ol, 17-amino-2-methoxy-, (17\beta)- (9CI)
CN
     INDEX NAME)
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10458286

RN 431901-69-8 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 3-hydroxy-2-methoxy-, oxime (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 431901-70-1 CAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431901-71-2 CAPLUS

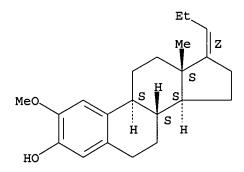
CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-methyl-, (17 β)- (9CI) (CA INDEX NAME)

RN 431901-72-3 CAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 2-methoxy-17-propylidene-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

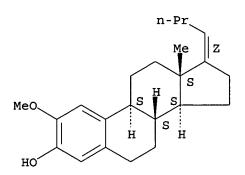


RN 431901-77-8 CAPLUS

CN 19,21-Dinorchola-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.



RN 431901-78-9 CAPLUS

CN 19,21-Dinorchola-1,3,5(10)-trien-3-ol, 2-methoxy- (9CI) (CA INDEX NAME)

RN 431901-80-3 CAPLUS

CN Estra-1,3,5(10)-triene-16-carboxylic acid, 2-methoxy-17-oxo-3-(phenylmethoxy)-, methyl ester, (16α) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431901-89-2 CAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 2-amino- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431901-90-5 CAPLUS

CN Estra-1,3,5(10)-trien-3-ol, 2-(dimethylamino)- (9CI) (CA INDEX NAME)

10458286

RN 431901-91-6 CAPLUS

CNFormamide, N-(3-hydroxyestra-1,3,5(10)-trien-2-yl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN431901-92-7 CAPLUS

Estra-1,3,5(10)-trien-3-ol, 2-(methylamino)- (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

RN431901-93-8 CAPLUS

Estra-1,3,5(10)-trien-3-ol, 2-azido- (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

431901-98-3 CAPLUS RN

CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-methyl-,

 $(16\alpha, 17\beta)$ - (9CI) (CA INDEX NAME)

RN 431901-99-4 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-methyl-, $(16\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431902-01-1 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 16-(hydroxymethyl)-2-methoxy-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431902-02-2 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 16-(hydroxymethyl)-2-methoxy-, (16β,17β)- (9CI) (CA INDEX NAME)

RN 431902-03-3 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-propyl-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431902-04-4 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-propyl-, $(16\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431902-05-5 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 16-butyl-2-methoxy-, $(16\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 431902-06-6 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-(2-methylpropyl)-, (16β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 438044-30-5 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 16-[(dimethylamino)methyl]-2-methoxy-, (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 464924-32-1 CAPLUS CN Estra-1,3,5(10)-triene-16-methanol, 17-hydroxy-2-methoxy-3-(phenylmethoxy)-, (17 β)- (9CI) (CA INDEX NAME)

RN 594873-85-5 CAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 16-[(dimethylamino)methyl]-2-methoxy-3-(phenylmethoxy)-, (16β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 594873-86-6 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-methyl-, (17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 594873-87-7 CAPLUS

CN 19-Norpregna-1,3,5(10),17(20)-tetraen-3-ol, 2-methoxy-, (17E)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

NPA

ANSWER 11 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN 2003:6101)98 CAPLUS

AN

139:159968 DN

Nonsteroidal analogs of 2-methoxyestradiol for the treatment of diseases ΤI characterized by undesirable angiogenesis, proliferative activity, or cell

Agoston, Gregory; Shah, Jamshed H.; Hunsucker, Kimberly A.; Treston, IN Anthony M.; Pribluda, Victor S.

PΑ

Entremed, Inc., USA PCT Int. Appl., 105 pp. so

CODEN: PIXXD2

DTPatent

LA English

FAN.CNT 2																					
	PATENT NO.)	DATE		APPLICATION NO.						DATE					
							-														
ΡI	WO	2003063787			A2		20030807			WO 2003-US2728						20030130					
	WO	2003	0637	87		A 3	3 20040122														
		W:	ΑE,	AG,	AL,	AM,	ΑT,	ΑŬ,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,			
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,			
			GM,	HR,	HU,	ID,	ΙL,	IN,	IS,	JP,	ΚE,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,			
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,			
			PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,			
			UA,	ŪĠ,	US,	UΖ,	VC,	VN,	YU,	ZA,	ZM,	ZW									
		RW:	GH,	GM,	ΚE,	LS,	MW,	MZ,	SD,	SL,	SZ,	ΤZ,	ŪĠ,	ZM,	ZW,	AM,	ΑZ,	BY,			
			KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	ΒE,	BG,	CH,	CY,	CZ,	DE,	DK,	EE,	ES,			
			FI,	FR,	GB,	GR,	HU,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	SI,	SK,	TR,	BF,			
			ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	ΝE,	SN,	TD,	TG				
	US	2003	1870	76		A1		2003	1002	1	US 2	003-	3549	21		2	0030	130			
	US	2003	2364	39		A1		20031225		1	US 2003-354927					20030130					
PRAI	US	2002	-354	046P		P		2002	0130												
os	MAI	RPAT	139:	1599	68																

GΙ

$$R^{10}$$
 R^{3}
 R^{3}

AB The invention provides compds., compns., and methods for treating disease states characterized by undesirable angiogenesis, proliferative activity, or cell mitosis by administering 2-methoxyestradiol nonsteroidal analogs I, II or III [R1 = (substituted) alkyl, (substituted) aryl; R2, R3 = H, halo, (substituted) alkyl, etc.]. Preparation of e.g. I (R1, R2 = Me; R3 = H) is described.

IT 573976-95-1D, derivs. 573979-27-8 573979-28-9

573979-29-0 573979-30-3 573979-35-8

573979-36-9 573979-37-0 573979-38-1

573979-39-2 573979-40-5 573979-41-6

573979-42-7 573979-43-8 573979-44-9

573979-45-0 573979-46-1

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(methoxyestradiol nonsteroidal analogs for treatment of diseases characterized by undesirable angiogenesis, proliferative activity, or cell mitosis)

RN 573976-95-1 CAPLUS

CN 2,3-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro- (9CI) (CA INDEX NAME)

RN 573979-27-8 CAPLUS

CN 2-Phenanthrenol, 8-ethyl-4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7,7-dimethyl- (9CI) (CA INDEX NAME)

RN 573979-28-9 CAPLUS

CN 2-Phenanthrenemethanol, 1-ethyl-1,2,3,4,4a,9,10,10a-octahydro-7-hydroxy-6-methoxy-2-methyl- (9CI) (CA INDEX NAME)

RN 573979-29-0 CAPLUS

CN 2-Phenanthrenol, 7-ethenyl-8-ethyl-4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{CH} = \text{CH}_2 \\ \text{Et} \end{array}$$

RN 573979-30-3 CAPLUS

CN 2-Phenanthrenol, 8-ethyl-4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7-methyl-7-(1-propenyl)- (9CI) (CA INDEX NAME)

RN 573979-35-8 CAPLUS

CN 2-Phenanthrenol, 7-ethyl-4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7,8-dimethyl- (9CI) (CA INDEX NAME)

10458286

RN 573979-36-9 CAPLUS

CN 2-Phenanthrenemethanol, 1,2,3,4,4a,9,10,10a-octahydro-7-hydroxy-6-methoxy- α ,1,2-trimethyl- (9CI) (CA INDEX NAME)

RN 573979-37-0 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7,8-dimethyl-7-(1-methylethenyl)- (9CI) (CA INDEX NAME)

RN 573979-38-1 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7,8-dimethyl-7-(1-methyl-1-propenyl)- (9CI) (CA INDEX NAME)

RN 573979-39-2 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7-methyl-8-propyl-(9CI) (CA INDEX NAME)

10458286

RN 573979-40-5 CAPLUS

CN 1-Phenanthrenepropanol, 1,2,3,4,4a,9,10,10a-octahydro-7-hydroxy-6-methoxy-2-methyl- (9CI) (CA INDEX NAME)

MeO
$$(CH_2)_3-OH$$

RN 573979-41-6 CAPLUS

CN 2-Phenanthrenol, 8-(3-butenyl)-4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \\ \text{CH}_2-\text{CH}_2-\text{CH} \\ \end{array}$$

RN 573979-42-7 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7-methyl-8-(3-pentenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{MeO} \\ \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{CH} \\ \end{array}$$

RN 573979-43-8 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7-methyl-7-propyl-(9CI) (CA INDEX NAME)

RN 573979-44-9 CAPLUS

CN 2-Phenanthrenemethanol, α -ethyl-1,2,3,4,4a,9,10,10a-octahydro-7-hydroxy-6-methoxy-1,2-dimethyl- (9CI) (CA INDEX NAME)

RN 573979-45-0 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7,8-dimethyl-7-(1-methylenepropyl)- (9CI) (CA INDEX NAME)

RN 573979-46-1 CAPLUS

CN 2-Phenanthrenol, 7-(1-ethyl-1-propenyl)-4b,5,6,7,8,8a,9,10-octahydro-3-methoxy-7,8-dimethyl- (9CI) (CA INDEX NAME)

L14 ANSWER 12 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:252155 CAPLUS

DN 139:78657

TI Novel 2-methoxyestradiol analogues with antitumor activity

AU Tinley, Tina L.; Leal, Rachel M.; Randall-Hlubek, Deborah A.; Cessac,

MA

James W.; Wilkens, Lynne R.; Rao, Pemmaraju N.; Mooberry, Susan L.

CS Departments of Physiology and Medicine, Southwest Foundation for Biomedical Research, San Antonio, TX, 78227, USA

SO Cancer Research (2003), 63(7), 1538-1549

CODEN: CNREA8; ISSN: 0008-5472

PB American Association for Cancer Research

DT Journal

LA English

2-Methoxyestradiol (2-ME2) is a natural estrogen metabolite that, while AB devoid of estrogenic effects, has both antiangiogenic and antitumor effects. 2-ME2 is currently being evaluated in Phase I and Phase II clin. trials for the treatment of multiple types of cancer. Novel analogs of 2-ME2 were tested for activities that predict antiangiogenic and antitumor effects. Selected analogs were tested for inhibitory activity against endothelial cell proliferation and invasion. The results show that these analogs are effective inhibitors of endothelial cell activities that may predict antiangiogenic activity, and one analog, 2-methoxy-14dehydroestradiol (14-dehydro-2-ME2), was 6-15-fold more potent than the parental compound in these assays. The analogs were also evaluated for inhibition of proliferation and cytotoxicity against multiple tumor cell lines and found to be potent and effective. 14-Dehydro-2-ME2 was approx. 15-fold more potent than 2-ME2 against various tumor cell lines, and 2-methoxy-15-dehydroestradiol was particularly effective against DU 145 and PC3 prostate cancer cell lines. In vivo antitumor activity was observed for the three analogs tested in the murine xenograft MDA-MB-435 model; however, 2-ME2 provided no antitumor activity in this trial. The two most effective analogs, 14-dehydro-2-ME2 and 2-methoxyestradiol- $15\alpha, 16\alpha$ -acetonide, provided 29.4% and 26.7% inhibition of tumor burden, resp. Mechanism of action studies indicate that the analogs cause mitotic spindle disruption, mitotic arrest, microtubule depolymn., and inhibition of the assembly of purified tubulin similar to the effects of 2-ME2. Consistent with antimitotics that inhibit the dynamic instability of tubulin and initiate apoptosis, these novel 2-ME2 analogs cause Bcl-2 phosphorylation and activation of mitogen-activated protein kinase signaling pathways.

IT 477951-76-1 477951-83-0

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(novel 2-methoxyestradiol analogs with antitumor activity in relation to signal transduction and mechanism of action)

RN 477951-76-1 CAPLUS

CN Estra-1,3,5(10),15-tetraene-3,17-diol, 2-methoxy-, (17β)- (9CI) (CF INDEX NAME)

Absolute stereochemistry.

RN 477951-83-0 CAPLUS

CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 2-methoxy-, cyclic 15,16-(1-methylethylidene acetal), $(15\alpha,16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 13 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
L14
ΑN
     2003:153417 CAPLUS
DN
     138:187528
TI
     Preparation of octahydrophenanthrenes as NMDA antagonists
IN
     Buschmann, Helmut Heinrich; Englberger, Werner Guenter; Przewosny,
     Michael; Sattlegger, Michael; Schick, Hans; Henkel, Birgitta
PA
     Gruenenthal GmbH, Germany
SO
     Ger. Offen., 14 pp.
     CODEN: GWXXBX
                                                                        NPA
DT
     Patent
     German
LΑ
FAN.CNT 1
                         KIND
                                           APPLICATION NO.
     PATENT NO.
                               DATE
                                                                  DATE
                                _____
                                            -----
PΙ
     DE 10140213
                         A1
                               20030227
                                           DE 2001-10140213
                                                                   20010816
     WO 2003016261
                         A1
                               20030227
                                           WO 2002-EP8866
                                                                  20020808
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
             CO, CR, CU, CZ, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM,
             HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
             LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL,
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PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG 20040602 EP 2002-794708 EP 1423353 Α1 20020808 AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK US 2004162432 US 2004-778380 A1 20040819 20040213 PRAI DE 2001-10140213 20010816 Α WO 2002-EP8866 W 20020808 os CASREACT 138:187528; MARPAT 138:187528

GΙ

AB Title compds. [I; R, R1, R2 = H, (branched) (saturated) acyclic group, (saturated)

cyclic group, alkylenearyl, alkyleneheteroaryl, halo, cyano, OR5, SR5, CHF2, CF3, NHR5, N(R5)2, NO2, SO2R5; R2 = oxo group; R3, R4 = H, (branched) (saturated) acyclic group, (saturated) cyclic group, alkylenearyl, alkyleneheteroaryl; or R3R4 = (CH2)2-7; R5 = (branched) (saturated) C1-12 acyclic group, C3-7 cyclic group, (hetero)aryl] and racemates, diastereoisomers or enantiomers thereof were prepared Thus, N,N-dimethyl-N-[(1R, 4aS,10aS)-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-ylmethyl]amine (preparation given) in MeCOEt was stirred with ClSiMe3 for 4.5 h at room temperature to give 66% N,N-dimethyl-N-[(1R, 4aS,10aS)-1,2,3,4,4a,9,10,10a-octahydrophenanthren-1-ylmethyl]amine hydrochloride. The latter at 10 μ M gave 46% inhibition of (3H)-(+)-MK801 binding, and at 10 mg/kg i.v. in mice 74% inhibition of phenylquinone-induced writhing.

IT 498546-57-9P 498546-64-8P 498546-68-2P 498546-75-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of octahydrophenanthrenes as NMDA antagonists)

RN 498546-57-9 CAPLUS

CN 1-Phenanthrenemethanamine, 1,2,3,4,4a,9,10,10a-octahydro-N,N-dimethyl-, hydrochloride, (1R,10aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 498546-64-8 CAPLUS

CN

1-Phenanthrenemethanamine, 1,2,3,4,4a,9,10,10a-octahydro-6-methoxy-N,N-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)

HCl

RN 498546-68-2 CAPLUS

CN 3-Phenanthrenol, 8-[(dimethylamino)methyl]-4b,5,6,7,8,8a,9,10-octahydro-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 498546-75-1 CAPLUS

CN 1-Phenanthrenemethanamine, 3-(1,1-dimethylethyl)-1,2,3,4,4a,9,10,10a-octahydro-N,N-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)

● HCl

IT 498546-53-5P 498546-62-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of octahydrophenanthrenes as NMDA antagonists)

RN 498546-53-5 CAPLUS

CN 1-Phenanthrenemethanamine, 1,2,3,4,4a,9,10,10a-octahydro-N,N-dimethyl-, (1R,10aS)-rel- (9CI) (CA INDEX NAME)

RN 498546-62-6 CAPLUS

CN 1-Phenanthrenemethanamine, 1,2,3,4,4a,9,10,10a-octahydro-6-methoxy-N,Ndimethyl- (9CI) (CA INDEX NAME)

$$\mathsf{MeO} \qquad \qquad \mathsf{CH}_2 - \mathsf{NMe}_2$$

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 14 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN L14

2003:22633 CAPLUS AN

DN 138:67085

ΤI Preparation of activators of non-genotropic estrogen-like signaling (ANGELS) for use in stimulating bone formation and treating other diseases

NPA

IN

Manolagas, Stavros C.; Katzenellenbogen, John A. Anabonix, Inc., USA; The Board of Trustees of the University of Arkansas PA

PCT Int. Appl., 125 pp. SO

CODEN: PIXXD2

DT Patent

English LΑ

FAN. CNT 1												N						
	PATENT NO.				KIND DATE		APPLICATION NO.			DATE								
PI	WO 2003002058						1	WO 2002-US18544					20020610					
	WO	2003	0020	58		C1		2003	0327									
	WO	2003	0020	58		A3	A3 20030828											
	WO	2003	0020	58		C2 20040708												
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
								DK,										
								IN,										
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
								SE,									-	-
			UA,	ŪĠ,	UZ,	VN,	YU,	ZA,	ZM,	ZW							•	•
		RW:						MZ,			SZ,	TZ,	UG,	ZM,	ZW,	AM,	AZ,	BY,
								TM,										
			GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF.	ВJ,	CF.	CG.	CI.	CM.	GA.
								NE,				·	•	•	•	•	•	•
	US	2003	•			-	•	•		•	US 2002-165380					20020607		
		1404																
								ES,										
								RO,					•	,	,	,	,	,
PRAI	US	2001	-			-			•	,	,							
		2002																
		2002																
OS MARPAT 138:67085									– •									

The inventors have discovered compds. that are Activators of AB

Non-Genotropic Estrogen-like Signaling (ANGELS). ANGELS compds. are small mols. that mimic the non-genotropic effects of estrogen and androgen but substantially lack their genotropic effects. For example, the inventors have discovered that ANGELS compds. stimulate the formation of bone but have little or no feminizing or masculinizing effects. In preferred embodiments, the ANGELS are an estrenediol, androstenediol, estranediol, androstanediol, nor-estrenediol, homo-estrenediol, seco-estrenediol, nor-androstenediol, homo-androstenediol, seco-androstenediol, nor-estranediol, homo-estranediol, seco-estranediol, nor-androstanediol, homo-androstanediol, seco-androstanediol, or a estratrienol. Pharmaceutical compns. containing the ANGELS are addnl. claimed.

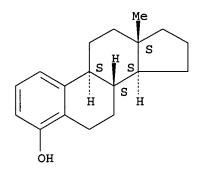
IT 481695-81-2DP, Estra-1,3,5(10)-trien-4-ol, analogs RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

> (preparation of activators of non-genotropic estrogen-like signaling (ANGELS) for use in stimulating bone formation and treating other diseases)

RN 481695-81-2 CAPLUS

CM Estra-1,3,5(10)-trien-4-ol (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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ANSWER 15 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
     2002:964373 CAPLUS
AN
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DN 138:24877

Preparation of novel 2-alkoxyestradiol analogs with antiproliferative and TI antimitotic activity

IN Rao, Pemmaraju Narasimha; Mooberry, Susan L.; Cessac, James W.; Tinley,

PA Southwest Foundation for Biomedical Research, USA

PCT Int. Appl., 86 pp. SO

CODEN: PIXXD2

DT Patent

LΑ English

FAN.	FAN.CNT 1																		
	PAT	CENT :	NO.			KIN	D	DATE		1	APPL	ICAT	ION I	NO.		D	ATE		
							-		- -		- 			-		-			
PI	WO	2002	1008	77		A1		2002	1219	1	WO 2	002-	US18	867		2	0020	511	
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KΕ,	KG,	ΚP,	KR,	ΚZ,	LC,	LK,	LR,	
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	ΝZ,	OM,	PH,	
			PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	ΤZ,	
			UA,	ŪĠ,	UΖ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,	KG,	ΚZ,	MD,	RU,	ТJ,	TM
		RW:	GH,	GM,	KE,	LS,	MW,	ΜZ,	SD,	SL,	SZ,	TZ,	ŪĠ,	ZM,	ZW,	ΑT,	BE,	CH,	
			CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	
			BF.	ВJ.	CF.	CG.	CI.	CM.	GA.	GN.	GO.	GW.	ML.	MR.	NE.	SN.	TD.	TG	

	US 2003096799	A1	20030522	US 2002-167208	20020611
	US 6593321	B2	20030715		
	US 2003229061	A1	20031211	US 2003-412007	20030411
PR	AI US 2001-297428P	P	20010611		
	US 2002-167208	A3	20020611		
os	MARPAT 138:24877				
GI					

$$R^{10}$$
 R^{20}
 R^{3}
 R^{3}
 R^{4}
 R^{5}
 R^{6}
 R^{6}
 R^{6}
 R^{10}
 R^{10}

AB Novel 2-alkoxyestradiol analogs of formula I [R1 = alkyl, haloalkyl; R2 = H, SO2NHR; R = H, alkyl, acyl; R3 = H, alkyl, haloalkyl; R4 = H, alkyl, alkenyl, alkynyl, aryl, heteroaryl; R5 = alkyl; R6 = O, NOR, OSO2NHR] are prepared which inhibit undesired cell proliferation and tumor growth. Addnl., methods are disclosed of treating diseases associated with undesired angiogenesis and undesired proliferation, and methods of treating infectious disease wherein the infectious agent is particularly susceptible to inhibition by agents that disrupt microtubule organization and function. Thus, II was prepared from estradiol in several steps. II was 6-24 times more potent than 2-methoxyestradiol in 5 human tumor cell lines.

IT 477951-76-1P

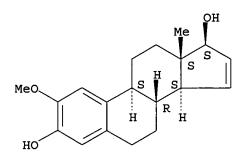
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of alkoxyestradiol analogs with antiproliferative and antimitotic activity)

RN 477951-76-1 CAPLUS

CN Estra-1,3,5(10),15-tetraene-3,17-diol, 2-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 477951-83-0P 477951-84-1P 477951-90-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of alkoxyestradiol analogs with antiproliferative and antimitotic activity)

RN 477951-83-0 CAPLUS

CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 2-methoxy-, cyclic 15,16-(1-methylethylidene acetal), $(15\alpha,16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-84-1 CAPLUS CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 2-methoxy-, cyclic 15,16-(1-methylethylidene acetal), (15 β ,16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-90-9 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-7-methyl-, $(7\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 477951-70-5P 477951-71-6P 477951-72-7P
477951-73-8P 477951-74-9P 477951-75-0P
477951-79-4P 477951-80-7P 477951-81-8P
477951-82-9P 477951-85-2P 477951-86-3P
477951-87-4P 477951-88-5P 477951-89-6P
477951-91-0P 477951-92-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)

(preparation of alkoxyestradiol analogs with antiproliferative and antimitotic activity)

RN 477951-70-5 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 2-methoxy-3-(phenylmethoxy)-, cyclic 1,2-ethanediyl acetal (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-71-6 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 3-hydroxy-2-methoxy-, cyclic 1,2-ethanediyl acetal (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-72-7 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 3-(acetyloxy)-2-methoxy-, cyclic 17-(1,2-ethanediyl acetal) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-73-8 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 3-(acetyloxy)-16-bromo-2-methoxy-, cyclic

17-(1,2-ethanediyl acetal), (16 α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-74-9 CAPLUS

CN Estra-1,3,5(10),15-tetraen-17-one, 3-(acetyloxy)-2-methoxy-, cyclic 17-(1,2-ethanediyl acetal) (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-75-0 CAPLUS

CN Estra-1,3,5(10),15-tetraen-17-one, 3-hydroxy-2-methoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-79-4 CAPLUS

CN Estra-1,3,5(10),15-tetraene-3,17-diol, 2-methoxy-, diacetate, (17β) -(9CI) (CA INDEX NAME)

RN 477951-80-7 CAPLUS

CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 2-methoxy-, 3,17-diacetate, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-81-8 CAPLUS

CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 2-methoxy-, tetraacetate, $(15\alpha,16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-82-9 CAPLUS

CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 2-methoxy-, $(15\alpha,16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

RN 477951-85-2 CAPLUS

CN Ethanone, 1-[$(7\alpha,17\beta)$ -17-(acetyloxy)-3-hydroxy-7-methylestra-1,3,5(10)-trien-2-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-86-3 CAPLUS

CN Ethanone, $1-[(7\alpha,17\beta)-17-(acetyloxy)-7-methyl-3-(phenylmethoxy)estra-1,3,5(10)-trien-2-yl]-(9CI) (CA INDEX NAME)$

Absolute stereochemistry.

RN 477951-87-4 CAPLUS

CN Estra-1,3,5(10)-triene-2,17-diol, 7-methyl-3-(phenylmethoxy)-, diacetate, $(7\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

RN 477951-88-5 CAPLUS CN Estra-1,3,5(10)-triene-2,17-diol, 7-methyl-3-(phenylmethoxy)-, $(7\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-89-6 CAPLUS CN Estra-1,3,5(10)-trien-17-ol, 2-methoxy-7-methyl-3-(phenylmethoxy)-, $(7\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 477951-91-0 CAPLUS CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 2-methoxy-, tetraacetate, $(15\beta,16\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 477951-92-1 CAPLUS

CN Estra-1,3,5(10)-triene-3,15,16,17-tetrol, 2-methoxy-, $(15\beta,16\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 16 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:778714 CAPLUS

DN 137:279370

TI Preparation of 2-methoxyestradiol derivatives as antiangiogenic agents

IN Agoston, Gregory E.; Pribluda, Victor; Treston, Anthony M.; Green, Shawn J.

PA USA

SO U.S. Pat. Appl. Publ., 15 pp. CODEN: USXXCO

DT Patent

LA English

FAN.CNT 1

1141.	C11 1						
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
PI	US 2002147183	A1	20021010	US 2001-779331	20010208		
PRAI	US 2001-779331		20010208				
os	CASREACT 137:279370	; MARPA	r 137:279370				
GI							

Derivs. of 2-methoxyestradiol of formula I [R1, R4 = H, halo, CN, alkyl, OH, CH2OH, NH2, etc.; R2 = N3, CN, alkynyl, alkenyl, alkoxy, etc.; R3 = H, OH, hydroxyalkyl, etc.; R5 = H, oxo, OH, NOH, etc.; R6, R7 = H, alkyl, alkenyl, alkynyl, etc.; R8 = OH, oxo, NOH, etc.] are prepared for the treatment of mammalian disease characterized by undesirable angiogenesis. Thus, II was prepared from 2-methoxyestradiol, and had IC50 of <0.5 μM against MDA-MB-231 human breast carcinoma cells.

Ne

1T 431901-87-0P 431901-98-3P 431901-99-4P 431902-00-0P 431902-01-1P 431902-02-2P 431902-03-3P 431902-04-4P 431902-05-5P 431902-06-6P 438044-30-5P

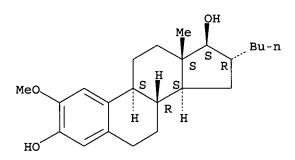
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 2-methoxyestradiol derivs. as antiangiogenic agents) 431901-87-0 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 16-butyl-2-methoxy-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN



RN 431901-98-3 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-methyl-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431902-00-0 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 16-ethyl-2-methoxy-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431902-01-1 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 16-(hydroxymethyl)-2-methoxy-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431902-02-2 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 16-(hydroxymethyl)-2-methoxy-, $(16\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 431902-03-3 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-propyl-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431902-04-4 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-propyl-, $(16\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431902-05-5 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 16-butyl-2-methoxy-, $(16\beta,17\beta)$ - (9CI) (CA INDEX NAME)

RN 431902-06-6 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-16-(2-methylpropyl)-, (16β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 438044-30-5 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 16-[(dimethylamino)methyl]-2-methoxy-, (16 β ,17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

Double bond geometry unknown.

RN 431901-82-5 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 2-methoxy-3-(phenylmethoxy)-16-(2-propenyl)-, (16 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 431901-85-8 CAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 16-(2-butenyl)-2-methoxy-3-(phenylmethoxy)-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 464924-28-5 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 16-(2-butenyl)-2-methoxy-3-(phenylmethoxy)-, (16β) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 464924-29-6 CAPLUS

CN Estra-1,3,5(10)-triene-16-carboxylic acid, 2-methoxy-17-oxo-3-(phenylmethoxy)-16-(2-propenyl)-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 464924-30-9 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 16-[(dimethylamino)methyl]-2-methoxy-3-(phenylmethoxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 464924-31-0 CAPLUS

CN Estra-1,3,5(10)-triene-16-carboxylic acid, 2-methoxy-17-oxo-3-(phenylmethoxy)-, methyl ester (9CI) (CA INDEX NAME)

RN464924-32-1 CAPLUS

Estra-1,3,5(10)-triene-16-methanol, 17-hydroxy-2-methoxy-3-(phenylmethoxy)-CN, (17β) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 17 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN L14

AN 2002:521687 CAPLUS

DN 137:93613

Preparation of phenanthrenes for therapeutic use as estrogen receptor ΤI

ligands
Koehler, Konrad; Henssen, Cecilia; Nilsson, Marita; Gillner, Mikael; Liu,
Robert R.: Ratcliffe, Ronald W. IN

PΑ Karo Bio A.B., Swed.; Merck & Co., Inc.; et al.

so PCT Int. Appl., 138 pp.

CODEN: PIXXD2

DTPatent

LΑ English

FAN.CNT 1

ran.	PATENT NO.				KIND DATE			APPLICATION NO.					DATE		
PI	WO 200	205352	2	A2	2002	0711	WO	2001-	EP152	230		20	00112	224	
	WO 200	205352	2	A3	2004	0108									
	W:	AE,	AG, AL,	AM,	AT, AU,	ΑZ,	BA, BE	3, BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,	
		CO,	CR, CU,	CZ,	DE, DK,	DM,	DZ, EC	C, EE,	ES,	FI,	GB,	GD,	GE,	GH,	
		GM,	HR, HU,	ID,	IL, IN,	IS,	JP, KE	E, KG,	ΚP,	KR,	KZ,	LC,	LK,	LR,	
					MA, MD,										
					SD, SE,										
					YU, ZA,					•	•	•	•		
	RW	: GH,	GM, KE,	LS,	MW, MZ,	SD,	SL, SZ	Z, TZ,	ŪĠ,	ZM,	ZW,	AM,	ΑZ,	BY,	
		KG,	KZ, MD,	RU,	TJ, TM,	ΑT,	BE, CH	I, CY,	DE,	DK,	ES,	FI,	FR,	GB,	
		GR,	IE, IT,	LU,	MC, NL,	PT,	SE, TF	R, BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	
		GN,	GQ, GW,	ML,	MR, NE,	SN,	TD, TO	3		-	-	-	-	•	
	CA 243	3828		AA	2002	0711	CA	2001-	24338	328		20	00112	224	
	EP 139	9406		A2	2004	0324	EP	2001-	27266	53		20	0112	224	
	R:	AT,			DK, ES,										
					FI, RO,				-		•	·	·	•	

as

CN

		JP 2004523508	T2	20040805	JP 2002-554641	20011224
		US 2004127576	A1	20040701	US 2004-250521	20040120
F	PRAI	GB 2001-163	Α	20010104		
		GB 2001-164	Α	20010104		
		GB 2001-6434	Α	20010315		
		WO 2001-EP15230	W	20011224		
C	S	MARPAT 137:93613				
G	βI					

Phenanthrenes, such as I [R1 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl; R1 ≠ Ph; R1, R3 = oxo, thioxo, H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl; R4, R10a = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, aryl; R4a = H, Me, Et, etc.; 1,10-, 1,2-, 2,3-saturated or -unsatd.], were prepared for pharmaceutical use

estrogen receptor modulators for the treatment or prevention of a variety of conditions related to estrogen functioning including bone loss, bone fractures, osteoporosis, cartilage degeneration, endometriosis, uterine fibroid disease, hot flashes, increased levels of LDL cholesterol, cardiovascular disease, impairment of cognitive functioning, cerebral degenerative disorders, restenosis, gynecomastia, autoimmune disease, vascular smooth muscle cell proliferation, obesity, incontinence, and cancer of the lung, colon, breast, uterus, and prostate. Thus, phenanthrenone II was prepd in five steps starting from MeO-3-C6H4I. The prepared phenanthrenes were assayed for estrogen receptor binding activity with binding affinities for the α - and β -subtypes in the range of IC50 3 to 10,000 nM. Pharmaceutical compns. of the phenanthrenes were also presented.

IT 441330-80-9P 441330-85-4P 441330-86-5P 441330-89-8P 441330-90-1P 441330-94-5P 441330-95-6P 441330-99-0P 441331-01-7P 441331-03-9P 441331-11-9P 441331-13-1P 441331-18-6P 441331-20-0P 441331-26-6P 441331-36-8P 441331-38-0P 441331-71-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation of phenanthrenes for therapeutic use as selective estrogen receptor modulators)

RN 441330-80-9 CAPLUS

3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

RN 441330-85-4 CAPLUS

CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-hydroxy-, (1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441330-86-5 CAPLUS

CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-hydroxy-, (1R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441330-89-8 CAPLUS

CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-, (1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

RN 441330-90-1 CAPLUS
CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 1'-butyl1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-, (1'R,4'aR,10'aR)-rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.

RN 441330-94-5 CAPLUS
CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-hydroxy-2-methyl, (1R,2S,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441330-95-6 CAPLUS
CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-hydroxy-2-methyl, (1R,2R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

RN 441330-99-0 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-1-(3-methylbutyl)-, (1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-01-7 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-1-(2-phenylethyl)-, (1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-03-9 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-2,10a-dimethyl-1-(3-methylbutyl)-, (1R,2S,4aR,10aR)-rel-(9CI) (CA INDEX NAME)

RN 441331-11-9 CAPLUS

CN 3(2H)-Phenanthrenone, 10a-ethyl-1,4,4a,9,10,10a-hexahydro-7-hydroxy-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-13-1 CAPLUS

CN 3(2H)-Phenanthrenone, 10a-ethyl-1,4,4a,9,10,10a-hexahydro-7-hydroxy-1-(3-methylbutyl)-, (1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-18-6 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-4-phenyl-, (4R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

RN 441331-20-0 CAPLUS

CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-1'-(2-phenylethyl)-, (1'R,4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-26-6 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-1-(3-methylbutyl)-, (1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-36-8 CAPLUS

CN Spiro[cyclobutane-1,3'(2'H)-phenanthren]-2-one, 1',4',4'a,9',10',10'a-hexahydro-7'-hydroxy-10'a-methyl-, (1R,4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-71-1 CAPLUS
CN 2(1H)-Phenanthrenone, 3,4,4a,9,10,10a-hexahydro-7-hydroxy-4a-methyl-,
(4aR,10aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

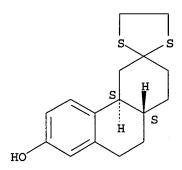
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RN

CN

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441331-37-9P 441331-39-1P 441331-41-5P
441331-42-6P 441331-43-7P 441331-44-8P
441331-45-9P 441331-46-0P 441331-48-2P
441331-49-3P 441331-55-1P 441331-62-0P
441331-65-3P 441331-66-4P 441331-69-7P
441331-70-0P 441331-72-2P 441331-73-3P
441331-74-4P 441331-75-5P 441331-76-6P
441348-21-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (preparation of phenanthrenes for therapeutic use as selective estrogen
   receptor modulators)
441330-81-0 CAPLUS
Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-
hexahydro-, (4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)
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Relative stereochemistry.



RN 441330-87-6 CAPLUS
CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 1'-butyl1',4',4'a,9',10',10'a-hexahydro-, (1'R,4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441330-91-2 CAPLUS CN 2-Phenanthrenol, 8-butyl-4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-, (4bR,8R,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441330-96-7 CAPLUS
CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-hydroxy-4-methyl, (1R,4S,4aS,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441330-97-8 CAPLUS CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 1'-butyl-1',4',4'a,9',10',10'a-hexahydro-2'-methyl-, (1'R,2'R,4'aS,10'aS)-rel-(9CI) (CA INDEX NAME)

RN 441330-98-9 CAPLUS
CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 1'-butyl1',4',4'a,9',10',10'a-hexahydro-2'-methyl-, (1'R,2'S,4'aS,10'aS)-rel(9CI) (CA INDEX NAME)

Relative stereochemistry.

Relative stereochemistry.

RN 441331-02-8 CAPLUS
CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-2,10a-dimethyl-1-(3-methylbutyl)-, (1R,2R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

RN 441331-04-0 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-6,6-dimethoxy-8a-methyl-8-(3-methylbutyl)-, (4bR,8R,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-05-1 CAPLUS

CN Spiro[1,3-dioxolane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-1'-(3-methylbutyl)-, (1'R,4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-06-2 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-8-(3-methylbutyl)-, (4bR,8S,8aR)-rel- (9CI) (CA INDEX NAME)

RN 441331-07-3 CAPLUS

CN 2-Phenanthrenol, 6-(ethylthio)-4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-8-(3-methylbutyl)-, (4bR,6S,8R,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-08-4 CAPLUS

CN Spiro[1,3-dithiane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-1'-(3-methylbutyl)-, (1'R,4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

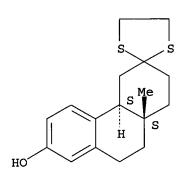
RN 441331-09-5 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

RN 441331-10-8 CAPLUS

CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-, (4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

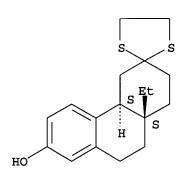
Relative stereochemistry.



RN 441331-12-0 CAPLUS

CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 10'a-ethyl-1',4',4'a,9',10',10'a-hexahydro-, (4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 441331-14-2 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-1-(3-methylbutyl)-, (1S,4aS,10aS)- (9CI) (CA INDEX NAME)

RN 441331-15-3 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-1-(3-methylbutyl)-, (1R,4aR,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 441331-16-4 CAPLUS

CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 10'a-ethyl-1',4',4'a,9',10',10'a-hexahydro-1'-(3-methylbutyl)-, (1'R,4'aR,10'aR)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

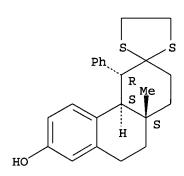
RN 441331-17-5 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-4a,10a-dimethyl-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

RN 441331-19-7 CAPLUS

CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-4'-phenyl-, (4'R,4'aS,10'aS)-rel- (9CI) (CA INDEX NAME)

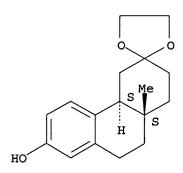
Relative stereochemistry.



RN 441331-21-1 CAPLUS

CN Spiro[1,3-dioxolane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-, (4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 441331-22-2 CAPLUS

CN Spiro[1,3-dioxolane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-, (4'aR,10'aS)-rel- (9CI) (CA INDEX NAME)

RN 441331-23-3 CAPLUS CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-pentyl-, (4bR,6R,8aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-24-4 CAPLUS CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-pentyl-, (4bR,6S,8aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-25-5 CAPLUS CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-2',10'a-dimethyl-1'-(3-methylbutyl)-, (1'R,2'S,4'aR,10'aR)-rel-(9CI) (CA INDEX NAME)

RN 441331-27-7 CAPLUS

CN Spiro[1,3-dithiane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-, (4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-28-8 CAPLUS

CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-hydroxy-4,10a-dimethyl-, (1R,4R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-29-9 CAPLUS

CN Spiro[1,3-dithiolane-2,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-4',10'a-dimethyl-, (4'R,4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

RN 441331-30-2 CAPLUS

CN 3 (2H) -Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-4-(phenylmethyl)-, (4R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-31-3 CAPLUS

CN 3 (2H) - Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-4,4-bis(phenylmethyl)-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-32-4 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-methylene-, (4bR,8aS)-rel- (9CI) (CA INDEX NAME)

RN 441331-33-5 CAPLUS

CN Spiro[cyclopropane-1,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-, (4'aR,10'aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-34-6 CAPLUS

CN Spiro[2,4-cyclohexadiene-1,3'(2'H)-phenanthren]-7'-ol, 2,3,4,5-tetrachloro-1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-, (1R,4'aS,10'aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

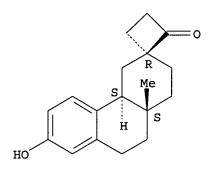
RN 441331-35-7 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-[1-(phenylthio)cyclopropyl]-, (4bR,6R,8aR)-rel- (9CI) (CA INDEX NAME)

RN 441331-37-9 CAPLUS

CN Spiro[cyclobutane-1,3'(2'H)-phenanthren]-2-one, 1',4',4'a,9',10',10'a-hexahydro-7'-hydroxy-10'a-methyl-, (1R,4'aS,10'aS)-rel- (9CI) (CA INDEX NAME)

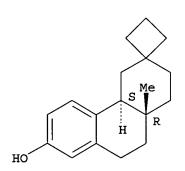
Relative stereochemistry.



RN 441331-39-1 CAPLUS

CN Spiro[cyclobutane-1,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-, (4'aR,10'aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



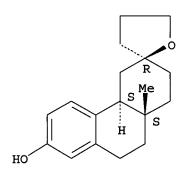
RN 441331-41-5 CAPLUS

CN Spiro[furan-2(3H),3'(2'H)-phenanthren]-7'-ol, 1',4,4',4'a,5,9',10',10'a-octahydro-10'a-methyl-, (2R,4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

RN 441331-42-6 CAPLUS

CN Spiro[furan-2(3H),3'(2'H)-phenanthren]-7'-ol, 1',4,4',4'a,5,9',10',10'a-octahydro-10'a-methyl-, (2R,4'aS,10'aS)-rel- (9CI) (CA INDEX NAME)

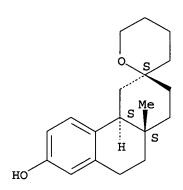
Relative stereochemistry.



RN 441331-43-7 CAPLUS

CN Spiro[phenanthrene-3(2H),2'-[2H]pyran]-7-ol, 1,3',4,4',4a,5',6',9,10,10a-decahydro-10a-methyl-, (2'R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 441331-44-8 CAPLUS

CN Spiro[phenanthrene-3(2H),2'-[2H]pyran]-7-ol, 1,3',4,4',4a,5',6',9,10,10a-decahydro-10a-methyl-, (2'R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

RN 441331-45-9 CAPLUS

CN Spiro[furan-2(3H),3'(2'H)-phenanthren]-7'-ol, 1',4,4',4'a,5,9',10',10'a-octahydro-10'a-methyl-1'-(3-methylbutyl)-, (1'R,2S,4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-46-0 CAPLUS

CN Spiro[cyclobutane-1,3'(2'H)-phenanthren]-7'-ol, 1',4',4'a,9',10',10'a-hexahydro-10'a-methyl-1'-(3-methylbutyl)-, (1'R,4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-48-2 CAPLUS

CN Spiro[furan-2(3H),3'(2'H)-phenanthren]-7'-ol, 1',4,4',4'a,5,9',10',10'a-octahydro-10'a-methyl-1'-(3-methylbutyl)-, (1'R,2R,4'aR,10'aR)-rel- (9CI) (CA INDEX NAME)

RN 441331-49-3 CAPLUS

CN 2(1H)-Phenanthrenone, 10a-butyl-3,4,4a,9,10,10a-hexahydro-7-hydroxy-4a-methyl-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-55-1 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-4b,8-dimethyl- (9CI) (CA INDEX NAME)

RN 441331-62-0 CAPLUS

CN 2(1H)-Phenanthrenone, 1-ethyl-3,4,4a,9,10,10a-hexahydro-7-hydroxy-4a-methyl-, (1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-65-3 CAPLUS

CN 2-Phenanthrenol, 8-butyl-4b, 5, 6, 7, 8, 8a, 9, 10-octahydro-4b-methyl-,

(4bR,8R,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-66-4 CAPLUS

CN 2-Phenanthrenol, 8-butyl-4b,5,6,7,8,8a,9,10-octahydro-4b-methyl-, (4bR,8S,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-69-7 CAPLUS

CN 2(1H)-Phenanthrenone, 4a-butyl-3,4,4a,9,10,10a-hexahydro-7-hydroxy-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-70-0 CAPLUS

CN 2(1H)-Phenanthrenone, 4a-butyl-3,4,4a,9,10,10a-hexahydro-7-hydroxy-, (4aR,10aS)-rel- (9CI) (CA INDEX NAME)

RN 441331-72-2 CAPLUS

CN Spiro[1,3-dithiolane-2,2'(1'H)-phenanthren]-7'-ol, 3',4',4'a,9',10',10'a-hexahydro-4'a-methyl-, (4'aR,10'aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-73-3 CAPLUS

CN 2(1H)-Phenanthrenone, 3,4,4a,9,10,10a-hexahydro-7-hydroxy-4a-methyl-, oxime, (4aR,10aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry unknown.

RN 441331-74-4 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-pentyl-, (4bR,6R,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-75-5 CAPLUS

CN 2-Phenanthrenol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-pentyl-, (4bR,6S,8aR)-rel- (9CI) (CA INDEX NAME)

RN 441331-76-6 CAPLUS

CN 2(1H)-Phenanthrenone, 1-ethyl-3,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-, (1R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441348-21-6 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-4-phenyl-, (4R,4aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 441332-20-3 441332-23-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of phenanthrenes for therapeutic use as selective estrogen receptor modulators)

RN 441332-20-3 CAPLUS

CN 2(1H)-Phenanthrenone, 3,4,4a,9,10,10a-hexahydro-7-methoxy-4a,10a-dimethyl-(9CI) (CA INDEX NAME)

RN 441332-23-6 CAPLUS
CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-10a-methyl-,
(4aR,10aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 441331-50-6P 441331-83-5P 441331-84-6P 441331-86-8P 441331-96-0P 441331-97-1P 441331-98-2P 441332-10-1P 441332-12-3P 441332-14-5P 441332-18-9P 441332-19-0P 441332-24-7P 441332-25-8P 441332-26-9P 441332-27-0P 441332-31-6P 441332-32-7P 441332-34-9P 441332-35-0P 441332-36-1P 441332-37-2P 441332-38-3P 441332-39-4P 441332-40-7P 441332-41-8P 441332-42-9P 441332-43-0P 441332-44-1P 441332-45-2P 441332-46-3P 441332-47-4P 441332-48-5P 441332-49-6P 441348-22-7P 441348-23-8P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of phenanthrenes for therapeutic use as selective estrogen receptor modulators) RN 441331-50-6 CAPLUS CN 2(1H)-Phenanthrenone, 10a-butyl-3,4,4a,9,10,10a-hexahydro-7-methoxy-4amethyl-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-83-5 CAPLUS CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-methoxy-,

(1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-84-6 CAPLUS

CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-methoxy-, (1R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-86-8 CAPLUS

CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-methoxy-10a-methyl-, (1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-96-0 CAPLUS

CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-methoxy-2-methyl-, (1R,2S,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

RN 441331-97-1 CAPLUS

CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-methoxy-2-methyl-, (1R,2R,4aS,10aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441331-98-2 CAPLUS

CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-7-methoxy-4-methyl-, (1R,4S,4aS,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-10-1 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-2,10a-dimethyl-1-(3-methylbutyl)-7-(phenylmethoxy)-, (1R,2R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

RN 441332-12-3 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-2,10a-dimethyl-1-(3-methylbutyl)-7-(phenylmethoxy)-, (1R,2S,4aR,10aR)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-14-5 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-10a-methyl-1-(3-methylbutyl)-7-(phenylmethoxy)-, (1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-18-9 CAPLUS

CN 3(2H)-Phenanthrenone, 10a-ethyl-1,4,4a,9,10,10a-hexahydro-1-(3-methylbutyl)-7-(phenylmethoxy)-, (1R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

RN 441332-19-0 CAPLUS

CN 2(1H)-Phenanthrenone, 3,4,4a,9,10,10a-hexahydro-7-methoxy-4a,10a-dimethyl-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-24-7 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-10a-methyl-7-(phenylmethoxy)-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-25-8 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-10a-methyl-7-(phenylmethoxy)-, (4aR,10aS)-rel- (9CI) (CA INDEX NAME)

RN 441332-26-9 CAPLUS

CN 3-Phenanthrenol, 1,2,3,4,4a,9,10,10a-octahydro-10a-methyl-3-pentyl-7-(phenylmethoxy)-, (3R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-27-0 CAPLUS

CN 3-Phenanthrenol, 1,2,3,4,4a,9,10,10a-octahydro-10a-methyl-3-pentyl-7-(phenylmethoxy)-, (3R,4aS,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-31-6 CAPLUS

CN 3(2H)-Phenanthrenone, 1-butyl-1,4,4a,9,10,10a-hexahydro-4,10a-dimethyl-7-(phenylmethoxy)-, (1R,4R,4aR,10aR)-rel-(9CI) (CA INDEX NAME)

RN 441332-32-7 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-7-hydroxy-4,10a-dimethyl-, (4R,4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-34-9 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-10a-methyl-7-(phenylmethoxy)-4,4-bis(phenylmethyl)-, (4aR,10aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-35-0 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-[1-(phenylsulfinyl)cyclopentyl]-, (4bR,8aR)-rel-(9CI) (CA INDEX NAME)

RN 441332-36-1 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-[3-(phenylmethoxy)propyl]-, (4bR,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-37-2 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-6-(3-hydroxypropyl)-8a-methyl-, (4bR,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-38-3 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-[3-[[(4-methylphenyl)sulfonyl]oxy]propyl]-, (4bR,6R,8aR)-rel- (9CI) (CA INDEX NAME)

RN 441332-39-4 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-[3-[[(4-methylphenyl)sulfonyl]oxy]propyl]-, (4bR,6S,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-40-7 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-6-(4-hydroxybutyl)-8a-methyl-, (4bR,6R,8aR)-rel- (9CI) (CA INDEX NAME)

RN 441332-41-8 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-6-(4-hydroxybutyl)-8amethyl-, (4bR,6S,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-42-9 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-[4-[[(4-methylphenyl)sulfonyl]oxy]butyl]-, (4bR,6R,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-43-0 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-6-[4-[[(4-methylphenyl)sulfonyl]oxy]butyl]-, (4bR,6S,8aR)-rel- (9CI) (CA INDEX NAME)

RN 441332-44-1 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-8-(3-methylbutyl)-6-[3-(phenylmethoxy)propyl]-, (4bR,6S,8R,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-45-2 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-6-(3-hydroxypropyl)-8a-methyl-8-(3-methylbutyl)-, (4bR,6S,8R,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-46-3 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-8-(3-methylbutyl)-6-[3-[[(4-methylphenyl)sulfonyl]oxy]propyl]-, (4bR,6S,8R,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-47-4 CAPLUS

CN 2,6-Phenanthrenediol, 4b,5,6,7,8,8a,9,10-octahydro-8a-methyl-8-(3-methylbutyl)-6-[1-(phenylthio)cyclopropyl]-, (4bR,6S,8R,8aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441332-48-5 CAPLUS

CN Spiro[cyclobutane-1,3'(2'H)-phenanthren]-2-one, 1',4',4'a,9',10',10'a-hexahydro-7'-hydroxy-10'a-methyl-1'-(3-methylbutyl)-, (1'R,4'aR,10'aR)-rel-(9CI) (CA INDEX NAME)

RN 441332-49-6 CAPLUS

CN Dispiro[1,3-dithiolane-2,1'-cyclobutane-2',3''(2''H)-phenanthren]-7''-ol, 1'',4'',4''a,9'',10'',10''a-hexahydro-10''a-methyl-1''-(3-methylbutyl)-, (1''R,4''aR,10''aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 441348-22-7 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-10a-methyl-1-(3-methylbutyl)-7-(phenylmethoxy)-, (1S,4aS,10aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 441348-23-8 CAPLUS

CN 3(2H)-Phenanthrenone, 1,4,4a,9,10,10a-hexahydro-10a-methyl-1-(3-methylbutyl)-7-(phenylmethoxy)-, (1R,4aR,10aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L14 ANSWER 18 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2002:122822 CAPLUS

DN 136:161698

TI Combination preparation with an $\text{ER}\beta$ selective estrogen and a SERM or antiestrogen

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Fritzemeier, Karl-Heinrich; Kollenkirchen, Uwe; Hegele-Hartung, Christa
TN
PΔ
     Schering Aktiengesellschaft, Germany
SO
     PCT Int. Appl., 33 pp.
     CODEN: PIXXD2
DT
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FAN.CNT 1
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     WO 2001-EP9008
                          W
     A novel medicament for the treatment of estrogen-deficient disease states
AΒ
     is disclosed. Said medicament is a combination preparation comprising an
     ER\beta-selective estrogen and an ER\alpha-selective antiestrogen or
     SERM (Selective Estrogen Receptor Modulator). The antiestrogen or SERM
     which is a component of the combination preparation is preferably selective for
     the periphery. The preparation is suitable for an organ-specific estrogen
     therapy and has clear advantages over conventional therapies. Due to the
     combination of ER\alpha-selective SERM and ER\beta-estrogen the preparation
     permits a complete protection against bone loss caused by estrogen
     deficiency. The components of the medicament also have a synergistic
     effect with respect to the inhibition of inflammation inducing genes, in
     particular in inflammatory disorders such as atherosclerosis and
     arthritis, or neurodegenerative diseases such as Alzheimers and multiple
     sclerosis. Furthermore, pos. effects on cognition and mood may be
     expected. The protective estrogen-like effects are achieved, with no
     expectation of proliferation effects on breasts or uterus.
IT
     397872-24-1D, Estra-1,3,5(10)-triene-3,16-diol, derivs.
     RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (combination preparation with an ER\beta selective estrogen and a SERM or
        antiestrogen)
RN
     397872-24-1 CAPLUS
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Estra-1,3,5(10)-triene-3,16-diol (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CN

US 2000-207370P

MARPAT 135:318608

WO 2001-EP4290

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RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ANSWER 19 OF 19 CAPLUS COPYRIGHT 2005 ACS on STN
L14
AN
     2001:763027 CAPLUS
     135:318608
DN
     Preparation of 8\beta-hydrocarbyl-substituted estratrienes for use as
ΤI
     selective estrogens
     Peters, Olaf; Hillisch, Alexander; Thieme, Ina; Elger, Walter;
IN
     Hegele-Hartung, Christa; Kollenkirchen, Uwe; Fritzemeier, Karl-Heinrich;
     Patchev, Vladimir
     Schering Aktiengesellschaft, Germany
PA
     PCT Int. Appl., 90 pp.
so
     CODEN: PIXXD2
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     Patent
LA
     German
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     PATENT NO.
                                  DATE
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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PRAI DE 2000-10019167 A
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20000526

20010412

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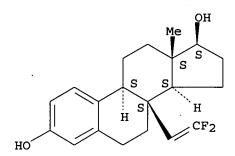
AΒ The invention relates to novel 8β -substituted estratrienes I [R2 = H, halogen, straight or branched (un) saturated C1-6-alkyl, alkoxy, CF3, sulfonamide; R3 = alkoxy, sulfonamide, acyloxy; R6, R7 = H; R6R7 = bond; R6', R7' = H, halogen, alkoxy, sulfonamide; R8 = a straight- or branched-chained, optionally partially or completely halogenated C1-5-alkyl, alkenyl, ethynyl, prop-1-ynyl; R9 = H, straight or branched (un) saturated C1-5-alkyl; R9R11 = bond; R11 = H; R11R12 = bond; R11' = H, halogen, a straight- or branched-chained, optionally partially or completely fluoro- or chloro-C1-4-alkyl, alkoxy, alkylthio; R12 = H; R14 = H; R14R15 = bond; R15 = H; R15R16 = bond; R15', R16' = H, halogen, alkoxy, sulfonamid; R16 = H; R17, R17' = H, H and halogen, H and OCH2Ph, H and sulfonamide, alkyl and acyl or acyloxy, alkoxy and alkyl, alkoxy and acyloxy; R17R17' = :CH2, :CR24R25; R24, R25 = halogen; R24R25 = 0]. Thus, vinylestradiol II was prepared from estra-1,3,5(10)-tetraenone III in 8 steps. The inventive estratrienes are used as pharmaceutically active substances that have in vitro a higher affinity to estrogen receptor prepns. of rat prostate than to estrogen receptor prepns. of rat uterus. and which in vivo preferably have a preferential effect on bone material as compared to uterus and/or a pronounced effect with respect to the stimulation of the expression of 5HT2a receptor and transporter. II showed a relative binding affinity for the estrogen receptor of 1 in rat uterus and of 83 in rat prostate. The invention further relates to the production of these novel compds., to their use in therapy and to the pharmaceutical forms of administration that contain said novel compds. The invention further describes the use of said compds. for treating estrogen-deficiency related diseases and conditions and to the use of an 8β-substituted estratriene structural part in the overall structures of compds. that are characterized by a dissociation in favor of their estrogen effect on the bone as compared to the uterus. ΙŢ

367264-79-7P 367264-81-1P 367264-83-3P 367264-92-4P 367929-02-0P 367929-03-1P 367929-08-6P, 8β-Ethyl-9β-estra-1,3,5(10)-triene-3,17β-ol 367929-16-6P 367929-17-7P 367929-18-8P 367929-19-9P 367929-20-2P 367929-21-3P 367929-22-4P 367929-23-5P 367929-24-6P 367929-25-7P 367929-26-8P 367929-27-9P 367929-28-0P 367929-29-1P

pw

Absolute stereochemistry.

Absolute stereochemistry.



RN 367264-83-3 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 8-(1Z)-1-propenyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 367264-92-4 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 8-(1E)-1-propenyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 367929-02-0 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-, (17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-03-1 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-, (17β)- (9CI) (CA INDEX NAME)

RN 367929-08-6 CAPLUS

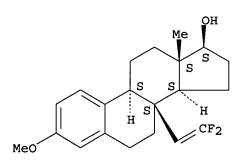
CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethyl-, $(9\beta,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-16-6 CAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 8-(2,2-difluoroethenyl)-3-methoxy-, (17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 367929-17-7 CAPLUS

CN Estra-1,3,5(10)-trien-17-ol, 8-ethyl-3-methoxy-, (17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-19-9 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-, 3-(acetylsulfamate), (17β) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-20-2 CAPLUS CN Estra-1,3,5(10)-trien-17-one, 3-[(aminosulfonyl)oxy]-8-ethenyl- (9CI) (CA INDEX NAME)

RN 367929-21-3 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 3-(acetyloxy)-8-ethenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-22-4 CAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, 8-ethenyl-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-23-5 CAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, 8-ethenyl-, 3-sulfamate, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

RN 367929-24-6 CAPLUS

CN Estra-1,3,5(10)-trien-17-one, 3-[(aminosulfonyl)oxy]-8-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-25-7 CAPLUS

CN Estra-1,3,5(10)-triene-3,16,17-triol, 8-methyl-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-26-8 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 8-propyl-, (17β)- (9CI) (CA INDEX NAME)

RN 367929-27-9 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethynyl-, (17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-28-0 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 16-fluoro-8-methyl-, $(16\alpha,17\beta)$ - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-29-1 CAPLUS

CN Estra-1,3,5(10)-triene-3,17-diol, 8-methyl-, (17 α)- (9CI) (CA INDEX NAME)

RN 367929-30-4 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-, diacetate, (17 β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

RN 367929-32-6 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-, 17-pentanoate, (17 β)- (9CI) (CA INDEX NAME)

RN 367929-33-7 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-, 17-acetate, (17β)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367929-34-8 CAPLUS CN Estra-1,3,5(10)-triene-3,17-diol, 8-ethenyl-, (9β,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Absolute stereochemistry.

RN 367264-74-2 CAPLUS

CN 2H-Pyran, 2-[[(17 β)-8-ethenyl-3-methoxyestra-1,3,5(10)-trien-17-yl]oxy]tetrahydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367264-75-3 CAPLUS

CN 2H-Pyran, 2-[[(17 β)-8-ethyl-3-methoxyestra-1,3,5(10)-trien-17-yl]oxy]tetrahydro- (9CI) (CA INDEX NAME)

RN 367264-80-0 CAPLUS

CN 2H-Pyran, 2-[[(17β)-8-(2,2-difluoroethenyl)-3-methoxyestra-1,3,5(10)-trien-17-yl]oxy]tetrahydro- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 367264-82-2 CAPLUS

CN 2H-Pyran, tetrahydro-2-[[(17 β)-3-methoxy-8-(1Z)-1-propenylestra-1,3,5(10)-trien-17-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 367264-91-3 CAPLUS

CN 2H-Pyran, tetrahydro-2-[[(17 β)-3-methoxy-8-(1E)-1-propenylestra-1,3,5(10)-trien-17-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

RN 367279-41-2 CAPLUS

CN Estra-1,3,5(10)-triene-8-carbonitrile, 11-hydroxy-3-methoxy-17- [(tetrahydro-2H-pyran-2-yl)oxy]-, (17β) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT